

# Resonant Tunneling in Disordered Materials such as SiO<sub>2</sub>/Si/SiO<sub>2</sub>

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**Abstract.** We have analyzed the effect of disorder in both the well and barriers of a resonant tunneling diode (RTD). If the disorder is limited solely to the barriers, a good peak-to-valley ratio (PVR) is expected. We describe a general guideline relating the PVR to the bulk mobility and effective mass of the well material of an RTD. We compare the effects of correlated versus uncorrelated disorder on the valley current. We discuss why interband tunnel devices such as the Esaki diode are more robust than RTDs in the presence of disorder.

## 1. Well versus Barrier Disorder

There have been a number of studies of Si / SiO<sub>2</sub> multilayer structures to look for quantization and resonant effects [1,2]. While the interface can be made smooth, the entire multi-layer structure is amorphous. Core level x-ray spectroscopy gives unambiguous evidence that quantization does occur, and that it follows the standard inverse square relationship to the well width [1]. However, there have been no strong demonstrations of resonant tunneling and negative differential resistance (NDR) in such systems. The observation of state-quantization with core-level-spectroscopy requires only conservation of total energy. State quantization is a necessary but not sufficient condition to observe NDR. Observation of NDR in an RTD requires conservation of both total energy and transverse momentum. The random potential resulting from the noncrystalline nature of the Si/SiO<sub>2</sub> material breaks the translational periodicity and, thus, the transverse momentum conservation required for high peak-to-valley ratios in RTDs.

We simulate the effect of the disorder by creating a mathematical model which mimics the macroscopic effects of amorphous disorder. The model gives the same momentum independence to the scattering since the correlation length of amorphous disorder is approximately the lattice constant, and the model gives the same bulk mobility. We begin with a single-band, tight-binding Hamiltonian which parameterizes the Si-Si (or for III-Vs, the cation-anion) basis matrix elements into a single number, the site energy. Then we assign a random component,  $\delta V$ , to the site energy. The random component has a Gaussian distribution with a mean of 0 and a variance of  $\sigma$ . The random component is uncorrelated between any two sites. The only free parameter in the model is  $\sigma$ . To relate  $\sigma$  to a physical quantity, we use the fact that the mobility resulting from this disorder is

$$\mu = \frac{4e\pi^{1/2}\hbar^4}{3m_c m_d^{3/2} (k_B T)^{1/2} \Omega \sigma^2} \quad (1)$$

where  $e$  is the magnitude of the electron charge,  $\Omega$  is the volume of the primitive cell,  $m_c$  is the conductivity effective mass and  $m_d$  is the density of states effective mass. The disorder is treated in the self-consistent Born approximation [3].

In Fig. (1), we choose the tight-binding parameters corresponding to an effective mass of 0.3 for the SiO<sub>2</sub> [4] and 0.5 for the a-Si [1]. In Fig. (1a) the disorder is restricted to the well region. We find that the NDR is destroyed when the mobility of the a-Si in the well is less than or equal to 250 cm<sup>2</sup>/Vs. If we take the same structure and restrict the same disorder to the barrier layers, there is almost no effect on the I-V and the PVR as is shown in Fig. (1b).

## 2. General Guideline Relating the PVR to the Bulk Mobility

When attempting to build an RTD in a new material system that is disordered or even amorphous, we would like to have some experimental measure which will predict whether the RTD will have a useful

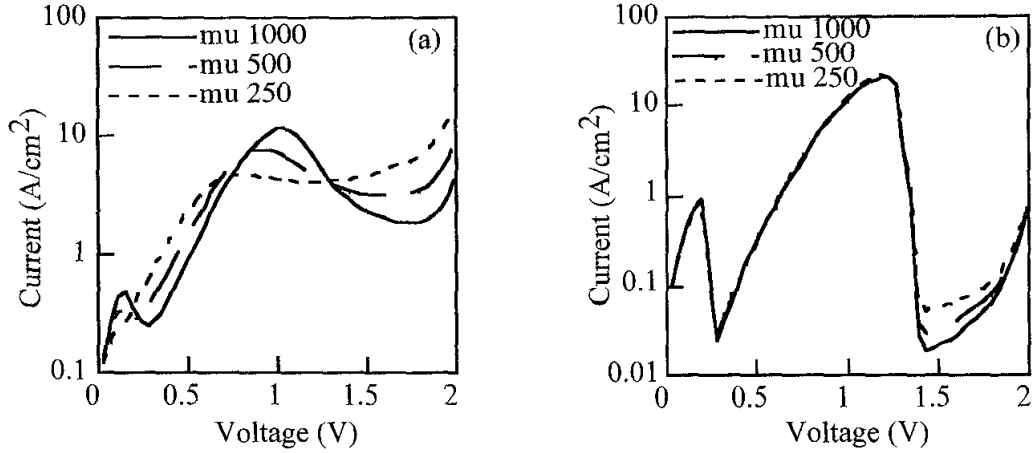


Figure 1. I-V of an amorphous  $\text{SiO}_2/\text{Si}/\text{SiO}_2$  RTD with dimensions 1.35/2.97/1.35 (nm) and  $10^{18} \text{ cm}^{-3}$  doped leads. (a) The disorder is restricted to the well region. (b) The disorder is restricted to the barrier region.

peak-to-valley ratio. We consider the case in which (a) both the mobility of the bulk material and the valley current of the RTD are determined by the static disorder scattering resulting from substitutional disorder (alloys), geometric disorder (amorphous and poly-crystalline materials), impurities and dopants, and (b) the bulk material and the thin layer have the same microscopic structure. Under such circumstances, both analytical [5] and numerical calculations show that the PVR is related to the bulk, room-temperature mobility by

$$\text{PVR} \propto \tau = \mu m_c / e. \quad (2)$$

Doping provides an experimental knob on the disorder and mobility. In a set of experiments, we increased the doping throughout an AlAs/InGaAs/AlAs based RTD, measured the PVR, and measured the mobility of the well material by growth of bulk InGaAs epi-layers characterized by resistivity and Hall measurements. We also numerically calculated the PVR of the InGaAs RTD as a function of mobility. The experimental and numerical results are shown in Fig. (2). Except at low mobility, the numerical calculations tend to underestimate the PVR. Therefore, we use the experimental data combined with relation (2) to make predictions for other materials.

We propose a general guide relating PVR to the bulk mobility and conductivity effective mass illustrated in Fig. (3). The PVR vs. mobility curve for the InGaAs RTD is replotted. The other curves are obtained by scaling the InGaAs mobility by  $m_{\text{InGaAs}}/m_{\text{new}}$ . The scaling law suggests that to obtain a PVR of 5 in a-Si with  $m_c \approx 0.5 m_0$  will require a mobility of  $400 \text{ cm}^2/\text{Vs}$ , well above values found for a-Si.

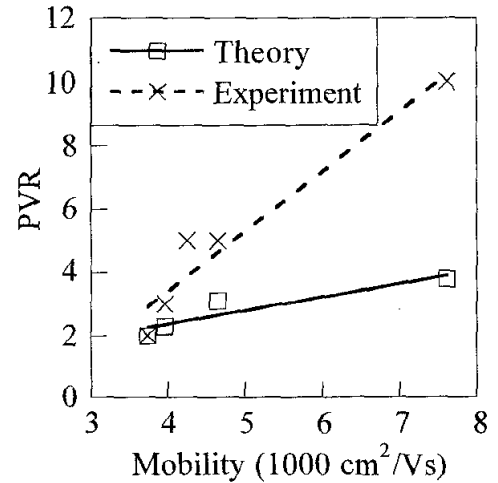


Fig. 2. Experimental and theoretical PVR vs. mobility for an InGaAs well.

### 3. Correlated Versus Uncorrelated Disorder

In an ideal epitaxial structure, the periodic crystal potential is undisturbed in the transverse plane, therefore transverse crystal momentum is conserved, and the process illustrated in Fig. (4) is not

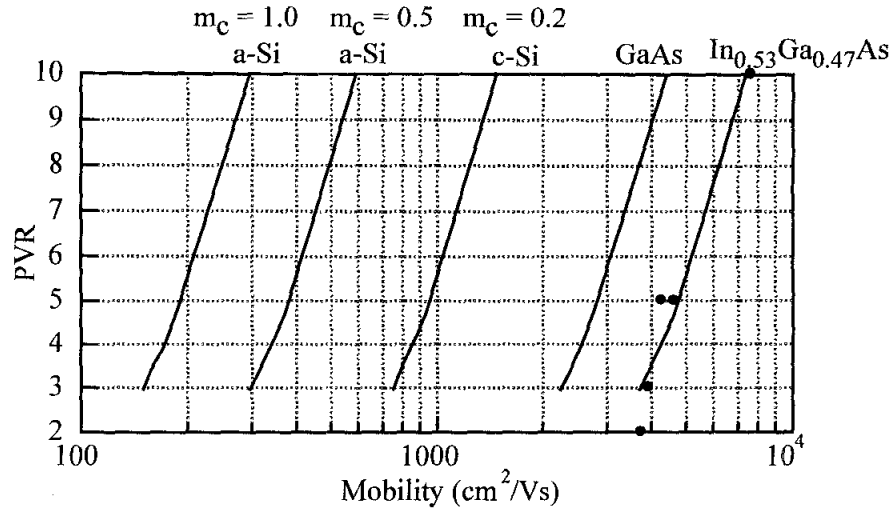


Figure 3. General guide relating PVR to the bulk mobility and conductivity effective mass of the well material.

allowed. In the presence of disorder, the incident electron can pick up a Fourier component of the disorder potential and scatter into a resonant transverse momentum state  $k_t^r$ . This is the process by which elastic scattering from disorder contributes to the valley current. The momentum coupling which determines the amount of momentum that an electron can obtain from the disorder is given by the Fourier transform of the random potential autocorrelation function.

When the disorder is uncorrelated  $\langle V(\mathbf{R})V(\mathbf{R}') \rangle \propto U\delta(\mathbf{R} - \mathbf{R}')$ , and the momentum coupling is a constant  $U$ . In this case, an incident electron can pick up any transverse momentum that it needs to get into the resonant state, and the scattering component of the valley current is nearly constant, independent of bias as illustrated schematically in Fig. (5a).

If the disorder is correlated, the inverse correlation length provides a cutoff to the momentum transfer. For example with Gaussian correlation,  $\langle V(\mathbf{R})V(\mathbf{R}') \rangle \propto e^{-|\mathbf{R}-\mathbf{R}'|^2/\Lambda^2}$  where  $\Lambda$  is the correlation length, and the momentum coupling falls off as  $|U_q|^2 \propto \Lambda^3 \pi^{3/2} e^{-q^2 \Lambda^2/4}$ . In the valley current region, as the bias is increased, an incident electron must pick up more transverse momentum to scatter into the resonant subband. The amount of momentum that the electron can obtain is governed by  $|U_q|^2$ . Therefore, for correlated disorder, the scattering component of the valley current falls off with bias as shown schematically in Fig. (5b).

We have numerically explored the effect of the correlation length for disorder limited to the interface layers of GaAs / AlAs RTDs for both exponentially and Gaussian correlated disorder [6]. Figs. (3) and (4) of reference [6] show that as the correlation length increases, the slope of the valley current region becomes more negative and the scattering assisted current decreases with bias. These results indicate that a polycrystalline well with large enough crystal sizes may be sufficient for observing NDR.

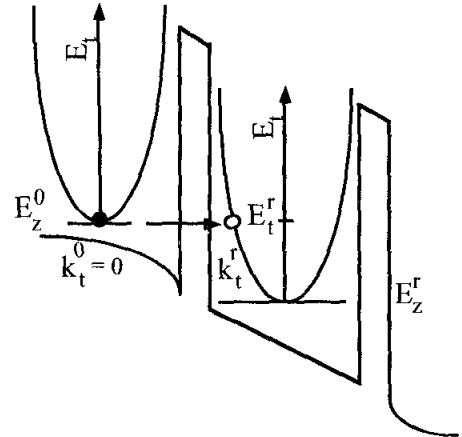


Figure 4. The parabolas represent the transverse kinetic energy. An off-resonant incident electron with longitudinal energy  $E_z^0$  and zero transverse kinetic energy can elastically scatter into the resonant state by trading off longitudinal energy for transverse kinetic energy.

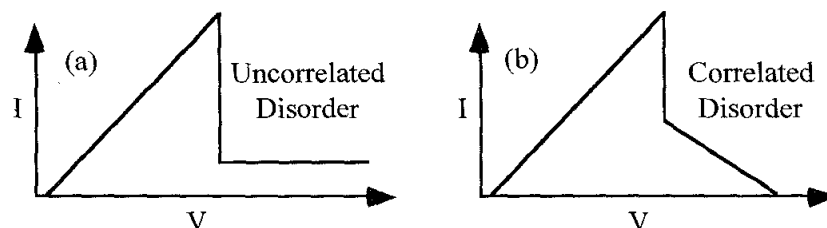


Figure 5. (a) The contribution to the valley current from uncorrelated disorder scattering is essentially flat, independent of bias. (b) The contribution to the valley current from correlated disorder scattering falls off with bias.

### Interband Tunnel Diodes and Disorder

Very general reasons suggest that an interband tunnel diode (ITD) such as the Esaki diode [7], the quantum well Esaki diode [8], or the resonant interband tunnel diode [9] should be less affected by disorder than an RTD. A notable difference between an ITD and an RTD is that an ITD requires one less conservation law to exhibit NDR. RTDs require conservation of both total energy and transverse momentum whereas ITDs require only conservation of total energy. For an RTD, Fig. 4 shows that there is always a high transverse-energy state in the well into which an incident electron can scatter while conserving total energy. For an ITD biased in the valley current region, there are no valence states into which an electron can elastically scatter (see for example Figs. (4), (6), and (8) of reference [10]). Since disorder scattering is elastic, the ITD should be more resilient than the RTD to the presence of disorder. This is in fact evident for an Esaki diode since the active region is doped to concentrations of  $10^{20} \text{ cm}^{-3}$ . Such a high doping in the well of an RTD would destroy its NDR.

### Summary

Although there is experimental evidence of coherent resonance effects in amorphous Si / SiO<sub>2</sub> materials, both numerical calculations and analytical theory do not show promise for good PVR from such materials. Amorphous barriers with a crystalline well, however, appear to be sufficient. The analysis of correlated disorder indicates that polycrystalline wells may be sufficient if the domain sizes are large enough. Interband devices are more robust in the presence of disorder since they require one less conservation law to work.

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